

**Final Report for Period:** 09/2010 - 08/2011**Submitted on:** 11/30/2011**Principal Investigator:** Yiacoumi, Sotira .**Award ID:** 0651683**Organization:** Georgia Tech Research Corp**Submitted By:**

Yiacoumi, Sotira - Principal Investigator

**Title:**

Like-Charge Electrostatic Attraction of Colloids in Aquatic Systems

**Project Participants****Senior Personnel****Name:** Yiacoumi, Sotira**Worked for more than 160 Hours:** Yes**Contribution to Project:****Name:** Tsouris, Costas**Worked for more than 160 Hours:** Yes**Contribution to Project:****Post-doc****Name:** Taboada-Serrano, Patricia**Worked for more than 160 Hours:** Yes**Contribution to Project:**

Patricia Taboada-Serrano participated in the project as a postdoctoral fellow. Her role was to develop molecular simulation techniques based on Monte-Carlo methods to study the interaction between colloidal particles and surfaces in aquatic systems.

**Name:** Hou, Chia-hung**Worked for more than 160 Hours:** Yes**Contribution to Project:**

Chia-hung Hou completed his PhD in May 2008 and continued participating in the project as a postdoctoral fellow. His role was to continue the development of molecular modeling techniques for colloidal particle and surface interactions and initiate the experiments for neutron reflectometry.

**Graduate Student****Name:** Hou, Chia-hung**Worked for more than 160 Hours:** Yes**Contribution to Project:**

Chia-hung Hou participated in the project as a graduate student. His role was to elucidate the electrical double layer formation near surfaces using molecular simulations and experimental techniques.

**Name:** Chung, Eunhyea**Worked for more than 160 Hours:** Yes**Contribution to Project:**

Eunhyea Chung participated in the project as a graduate student. Her role was to develop experimental techniques based on atomic force microscopy to measure the interaction between colloidal particles and surfaces. She also participated in developing computer codes and molecular simulations to estimate the interaction between colloidal particles and surfaces. In addition, she conducted neutron reflectometry experiments to better understand electrical double layer formation.

**Name:** Sharma, Ketki**Worked for more than 160 Hours:** Yes**Contribution to Project:**

Ketki Sharma participated in the project as a graduate student. Her role was to examine nanostructured materials for removing ionic pollutants from aqueous solutions and to develop molecular simulations for estimating the interaction between colloidal particles and surfaces. She also conducted neutron imaging experiments to quantify the diffusion of ions in nanostructured materials.

**Name:** Kweon, Hyojin

**Worked for more than 160 Hours:** Yes

**Contribution to Project:**

Hyojin Kweon participated in the project as a graduate student. Her role was to develop experimental techniques based on atomic force microscopy to measure interaction forces between colloidal particles and surfaces.

**Undergraduate Student**

**Name:** Lim, Mary

**Worked for more than 160 Hours:** Yes

**Contribution to Project:**

Mary Lim participated as an undergraduate student in the project in the fall semester of 2008 and spring semester of 2009. Her role was to characterize nanostructured materials and review the literature needed for neutron reflectometry experiments.

**Technician, Programmer**

**Other Participant**

**Research Experience for Undergraduates**

**Organizational Partners**

**Oak Ridge National Laboratory**

Neutron reflectometry and imaging experiments were conducted at the Spallation Neutron Source (SNS) and the High Flux Isotope Reactor (HFIR) of the Oak Ridge National laboratory (ORNL). Experiments at the Center for Nanophase Materials Sciences (CNMS) were also conducted to characterize materials and support molecular simulations on the electrical double layer formation near interfaces. Surface forces using radioactive materials were measured using an atomic force microscope located at ORNL. Furthermore, capacitive deionization experiments using nanostructured materials were conducted in collaboration with ORNL researchers.

**Other Collaborators or Contacts**

**Activities and Findings**

**Research and Education Activities:**

**Research Activities**

One of the main objectives of the project is to reveal the mechanisms involved in the electrostatic interaction between colloidal particles and surfaces in aquatic systems. The electrical double layer (EDL) plays an important role in determining the behavior of ionic species near charged surfaces. Molecular modeling based on Monte Carlo methods was developed to investigate the characteristics of EDL formation between two charged surfaces at the nanoscale, in which ion-ion interactions and ion size effects were taken into consideration.

Furthermore, Canonical Monte Carlo (CMC) simulations on the interaction of a charged spherical particle with a discretely charged surface in aqueous solutions containing single electrolytes and mixtures of electrolytes were performed to assess the effects of ion size and ion-ion correlations on interparticle interactions. These effects are neglected in the classical Derjaguin-Landau-Verwey-Overbeek (DLVO) theory via the consideration of ionic species as point charges with no interactions among themselves. Additionally, the DLVO theory assumes that

surface charge is uniform.

The choice of the geometry of the system seeks to replicate the geometry found in atomic force microscopy (AFM) in order to enable future comparison of modeling results and experimental data. In CMC simulations, long-range corrections are critical due to the small size of the simulation box. The size was optimized in this study so that the simulation time is minimized, while the box is large enough in order to ensure the formation of an EDL near the charged surface and bulk conditions far from it.

Canonical Monte Carlo simulations were also carried out to investigate the structure of EDL around a spherical colloidal particle. The minimum image criterion was employed for the ions in all directions. The periodic boundary conditions were not applied for the colloidal particle as the length of the simulation box was set large enough to neglect macroion-macroion interactions.

To explain colloidal interaction, the van der Waals force needs to be considered in addition to the electrostatic interaction. In this study, the van der Waals force between two colloidal particles was calculated as the sum of the interaction forces for every pair of molecules of the two objects. There have been many efforts to express the van der Waals interaction force since the 1930s. Macroscopically, the Hamaker approach or the Dzyaloshinskii-Lifshitz-Pitaevskii theory is used to estimate the van der Waals force, but the validity of the results is restricted by the range of parameters. This approach uses an approximation during integration of molecular forces, which makes it inaccurate when the particle is small. Based on a modified approach, the equation for the van der Waals force was improved in this project. With this approach, more accurate results are expected because the method does not use any approximations and is applicable to systems of various geometrical shapes that are difficult to be investigated by the Hamaker method.

Experiments to measure interaction forces between a colloidal particle and a flat surface were conducted using atomic force microscopy (AFM). Adhesion forces in both aquatic and atmospheric systems were measured with AFM in addition to more common force-distance curves. A variety of particles and surfaces were employed in the experiments. Experiments with silica particles, bacterial spores, such as *Bacillus thuringiensis*, and radioactive particles were conducted. Mica, gold, and radioactive gold surfaces were used. Also more traditional experiments based on cyclic voltammetry and sorption, as well as transport, of ions in nanostructured materials were carried out to better understand EDL formation near solid/liquid interfaces.

AFM experiments were conducted using a Multi Mode scanning probe microscope. Our AFM system has been upgraded with a Nanoscope V controller. This controller provides a higher resolution of the images, and the upgraded software includes a function called 'thermal tune' to measure the spring constant of a cantilever. The spring constant measurement is critical in obtaining an exact value of the interaction force.

Bacterial spore interactions with planar surfaces in aquatic environments, including adhesion forces and force-distance profiles, are influenced by the geometry and physicochemical properties of the system. The characteristics of spores of *Bacillus thuringiensis* (Bt) were determined using electron microscopy and electrokinetic measurements. The surface potentials of the spores and model surfaces used in the experiments were measured as a function of pH and ionic strength. The DLVO theory was employed to predict the interaction force between the spore and planar surfaces as a function of the separation distance, and a force balance was used to explain the adhesion force. Theoretical estimations were compared to experimental measurements obtained from AFM measurements.

One of the direct applications of the EDL in environmental processes is the removal of ionic species from aqueous solutions. Nanostructured materials, such as self-assembled mesoporous carbon (MC) materials synthesized at Oak Ridge National Laboratory, were examined for application in capacitive deionization (CDI) of saline water. MC was prepared by self-assembly of a triblock copolymer with hydrogen-bonded chains via a phenolic resin, such as resorcinol or phloroglucinol in acidic conditions, followed by carbonization and, in some cases, activation by KOH. Carbon synthesized in this way was ground into powder, from which activated MC sheets were produced. In a variation of this process, after the reaction of triblock copolymer with resorcinol or phloroglucinol, the gel that was formed was used to coat a graphite plate and then carbonized. The coated graphite plate was not activated and was tested to serve as current collector during the CDI process. The performance of these MC materials was compared to that of carbon aerogel for salt concentrations ranging between 1000 ppm and 35,000 ppm.

In another part of the study, EDL formation was studied by neutron reflectometry (NR). Early NR experiments to determine the ion concentration in the electrical double layer were unsuccessful because of the low concentration of ions. NR experiments conducted under this project were focused on the effects of the EDL on the distribution of nanometer-sized particles near a charged surface. These experiments were conducted at the Spallation Neutron Source (SNS, Oak Ridge, TN) on the variable wavelength Liquid Reflectometer. It was employed to study the interaction of nano-sized silica particles with a flat silica surface in aqueous solutions. The wavelength band used was 2.5–6 Å, with seven incident angles (0.15°, 0.25°, 0.45°, 0.65°, 0.85°, 1.6°, and 2.8°). Unlike other experimental tools that are used to study surface interactions, NR can provide information on the particle density profile in the solution near the interface. Two types of silica particles (25 nm and 100 nm) were suspended in aqueous solutions of varying pH and ionic strength.

Neutron imaging (NI) was also conducted at the High-Flux Isotope Reactor of the Oak Ridge National Laboratory (HFIR, Oak Ridge, TN). It

was employed as a tool to quantify the diffusion of ions inside nanostructured materials, such as mesoporous carbon electrodes. The focus was on mesoporous carbon materials of ~8-20 nm pore size, which are synthesized at Oak Ridge National Laboratory. The study of ion transport in porous materials is important in environmental and energy applications, such as desalination of water by capacitive deionization and energy storage in supercapacitors. Neutron imaging sequences of a specially designed electrochemical flow-through cell containing two mesoporous carbon electrodes were obtained under different conditions of applied potential. The images of the carbon electrodes acquired over time were coupled with transport modeling to provide the effective diffusion coefficient of ions in the electrodes. The diffusion coefficient of ions can be used to model the capacitive deionization process, as well as energy-storage devices.

### Education Activities

A course, Process Principles in Environmental Engineering, was offered to graduate students in Environmental Engineering at GIT, and another course, Environmental Engineering Systems, to undergraduate students in the School of Civil and Environmental Engineering at GIT. Both courses emphasize mathematical modeling of environmental systems. In addition, the graduate course was offered through the Distance Learning Program of GIT and, therefore, reached industrial researchers and practitioners. A section of the course, Civil Engineering Systems, which is required by all Civil and Environmental Engineering undergraduate students was also offered. This course introduces students to a sustainable engineering approach for planning, design, implementation, operation, and renewal of civil engineering systems.

This project supported the education of five students and two postdoctoral fellows. Chia-hung Hou was supported through the project and graduated with a Ph.D. degree in Environmental Engineering in 2008. He was a visiting student at the Oak Ridge National Laboratory (ORNL), using state-of-the-art equipment and experimental techniques needed in his research, and he continued working on the project as a postdoctoral fellow. Patricia Taboada-Serrano was partially supported through this project as a postdoctoral fellow, and then became a no-cost collaborator. Eunhyea Chung was supported through this project conducting related research for her Ph.D. dissertation and graduated with a Ph.D. degree in Environmental Engineering in 2011. She was also a visiting student at ORNL, using specialized equipment at the Center for Nanophase Materials Sciences needed in her research and participating in the neutron reflectometry experiments conducted at the Spallation Neutron Source. Ketki Sharma and Hyojin Kweon were supported through this project conducting research for their Ph.D. dissertations. Ketki Sharma was also a visiting student at Oak Ridge National Laboratory, using specialized experimental equipment and facilities needed in her research. She conducted capacitive deionization experiments, and participated in neutron imaging and reflectometry experiments conducted at the Spallation Neutron Source and the High Flux Isotope Reactor of the Oak Ridge National Laboratory. Mary Lim, who was introduced to the project with the objective to motivate her to pursue graduate studies in environmental engineering, conducted undergraduate research in Fall 2008 and Spring 2009.

### Findings:

Molecular simulation results indicated that electrical double layer (EDL) formation is not only determined by the ionic strength or the surface charge, but also by the ion size and charge. The competitive behavior between ion charge and size could result in the 'inversion' of the order between monovalent and multivalent counterions present in a mixture of electrolytes. It implies that these competitive effects not only determine the screening of surface charge but also significantly affect the electrolyte distribution within charged pores. Moreover, charge inversion takes place in the central region of nanopores because of the strong ion-ion correlations and the asymmetries in size and charge of ions (Hou et al., J. Chem. Phys., 2008a). Also, based on batch sorption experiments, the competition between ions that have different characteristics (i.e., charge and size) can further be observed using nanoporous carbon materials in an external electric field (Hou et al., J. Phys. Chem. B, 2008).

Grand canonical Monte Carlo simulations were employed to study the selective electrosorption of ions from a mixture of symmetric and asymmetric electrolytes confined in pores, and results were compared to experimental observations obtained via cyclic voltammetry and batch electrosorption equilibrium experiments (Hou et al., J. Chem. Phys., 2008b). Because of the competitive effects resulting from asymmetries in charge and size associated with different ions, the electrosorption selectivity of small monovalent over large divalent counterions first decreases with increasing surface charge, passes through a minimum, and then increases with further increase in surface charge. At low and moderate surface charge densities, the fact that large divalent counterions preferentially screen the surface charge has a strong effect on pore occupancy; whereas at a very high surface charge density, size-exclusion effects dominate and determine the accessibility of different ions into the pores. Therefore, electrosorption selectivity of ions from a mixture of electrolytes could, in principle, be achieved via tuning the electrical double-layer formation inside the pores through the regulation of surface charge tailored for different ion characteristics.

According to the Derjaguin-Landau-Verwey-Overbeek (DLVO) theory, the interaction force between two charged surfaces in solution is the sum of the van der Waals force and the electrostatic or EDL force. Thus, theoretical calculations can be used to model the interaction force between a gold electrode and a standard silicon-nitride cantilever tip measured by atomic force microscopy (AFM) (Taboada-Serrano et al., Ind. Eng. Chem. Res., 2008). The comparison between predicted interaction force values and those measured via AFM reveals that an effective electrode/electrolyte potential, rather than the applied potential to the electrode, should be considered to predict the electrostatic force between

a particle and an externally charged electrode in an aqueous solution. The association of ions present in solution with the solid/electrolyte interface, or the accumulation of ions next to the surface, determines the magnitude of the effective potentials at different conditions of pH and ionic strength.

Canonical Monte Carlo calculations of the electrostatic component of the interaction force between a charged spherical particle and a planar surface reveal the occurrence of two competing effects: minimization of energy vs. size exclusion or entropic effects. For example, it is energetically favorable for ions of the highest valence to preferentially neutralize the surface charge, and therefore be the main contributors to the electrostatic force between the particles. However, if the ions of higher valence are larger (in terms of size) than the low-valence ions, the low-valence ions preferentially neutralize surface charge. The low-valence ions in this case are mainly responsible for the direction and magnitude of the interaction force. Furthermore, strong correlation between ions bearing opposite charge results in ordering of fluid layers with higher local concentrations of ions of opposite sign in the enclosed space of the interacting surfaces. This ordering, which is stronger for ions of large size asymmetries, results in the presence of an attractive long-range force between surfaces that are likely charged, i.e., at certain separation distances like-charge attraction takes place mediated by the electrolyte solution. Additionally, a short-range minimum in the interaction force between likely-charge surfaces occurs almost at point of contact due to depletion effects. Real-sized ions are displaced from the increasingly small separation between surfaces as they approach to contact. Depletion effects are also more marked if the electrolyte solution contains large-sized ions.

The estimation of the van der Waals force using a modified approach in this study showed this force to be larger than that based on the Hamaker method. The van der Waals force is added to the electrostatic force in the simulations for a better comparison between molecular simulations and experimental data from AFM measurements. It was observed that the van der Waals potential is significant at a short separation distance between the colloidal particle and the charged surface. The van der Waals potential is inversely proportional to the sixth power of the distance between the objects while the electrostatic potential is inversely proportional to the second power of the distance. Therefore, the van der Waals potential is dominant at separation distances about 10 angstroms or less.

The results on molecular simulations of interaction forces between a planar surface and a charged spherical particle were presented at the 13th International Conference and Surface and Colloid Science (ICSCS)/83rd ACS Colloid and Surface Science Symposium held at Columbia University in New York City on June 14-19, 2009.

The van der Waals potential estimated by using the molecular approach can also be applied for atmospheric systems. The Hamaker constant is the only parameter that changes according to the medium type. Typically, the Hamaker constant in air is larger than that in aqueous solutions. The calculation of the van der Waals force was presented at the Chemical and Biological Defense Physical Science & Technology Conference held in New Orleans on November 17-21, 2008.

To obtain a better understanding of the electrostatic force, it was investigated as one of the components of the adhesion force between *Bacillus thuringiensis* (Bt) spores and planar surfaces in atmospheric systems. The surface potentials of a Bt spore and a mica surface were experimentally obtained using a combined AFM-scanning surface potential microscopy technique. On the basis of experimental information, the surface charge density of the spores was estimated at 0.03 microC/cm<sup>2</sup> at 20% relative humidity and decreases with increasing humidity. The Coulombic force was introduced for the spore-mica system (both charged, nonconductive surfaces), and an electrostatic image force was introduced to the spore-gold system because gold is electrically conductive. The Coulombic force for spore-mica is repulsive because the components are similarly charged, while the image force for the spore-gold system is attractive. The magnitudes of both forces decrease with increasing humidity. The electrostatic forces were added to other force components, e.g., van der Waals and capillary forces, to obtain the adhesion force for each system. The adhesion forces measured by AFM were compared to the estimated values. It was shown that the electrostatic (Coulombic and image) forces play a significant role in the adhesion force between spores and planar surfaces (Chung et al., Environ. Sci. Technol., 2010).

The interaction of Bt-spores and surfaces was also investigated in aquatic systems. For the Bt spore-mica surface system, force calculations using the DLVO theory showed a relatively good agreement with the experimental values. Therefore, it can be concluded that the van der Waals and electrostatic interaction forces play important roles in the interaction between a Bt spore and a planar surface in an aqueous solution, and the behavior of the spore is similar to the behavior of inorganic particles. A discrepancy observed between the theoretical force-distance curves and experimental results for the Bt spore-gold surface system was attributed to the approximate zeta potential values of the gold surface. Explaining the experimental force curve using the DLVO theory by modifying the zeta potential of the gold surface provided zeta potential values that described better the force measurements. These results were presented at the 85th ACS Colloid and Surface Science Symposium held at McGill University in Montreal, Canada on June 19-22, 2011 and submitted for publication in a peer-reviewed journal.

Our work on surface interaction forces has been extended to radioactive aerosol particles. In this part of the study, atomic force microscopy (AFM) was employed to quantify surface forces between a particle and a planar surface and to compare measurements with and without the involvement of radioactivity. The main objective of this work was to assess directly the effects of radioactivity on the surface interactions of

radioactive aerosols via the measurement of the adhesion force. The adhesion force between a silicon nitride AFM tip and an activated gold substrate was measured so that any possible effects due to radioactivity could be observed. The adhesion force between the tip and the gold surface increased significantly when the gold substrate (25 mm<sup>2</sup> surface area) was activated to a level of approximately 0.6 mCi. The results were explained by means of the image electrostatic force. The results of this investigation prompted further work under a different project into the effects of radioactivity in particle-surface interactions. (Walker et al., *J. Colloid Interf. Sci.*, 2010).

Nanostructured materials were employed to remove ionic pollutants from aqueous solutions for application in capacitive deionization (CDI) of saline water. In the CDI experiments, mesoporous carbon (MC) performed much better than carbon aerogel under the conditions of the experiment. It was associated with 25% drop in conductivity as compared to 2% drop in conductivity for carbon aerogel. The MC-coated graphite, both resorcinol (R) and phloroglucinol (P) type, has a higher capacity for ions than carbon aerogel. The salt removal capacity of RMCG-FS and PMCG-FS at 5000 ppm Instant Ocean concentration was 13.8 and 12.4 mg/g of carbon, respectively. The effect of salt concentration on the CDI performance of activated MC sheets was also examined for initial salt concentration of 1000, 3000, and 5000 ppm Instant Ocean solutions. The highest removal efficiency was observed at 3000 ppm concentration. The RMCG-FS electrodes showed the highest mass of salt removed at salt concentrations in the range of 4000 ppm. The results indicate that the MC-coated graphite electrodes can be used to deionize solutions of high concentration. Further experiments were carried out to compare the performance of RMCG-FS and carbon aerogel and observe the influence of temperature on the performance of both the materials. RMCG-FS exhibited a 34% higher ion removal capacity over carbon aerogel, along with more efficient removal at a higher temperature. (Tsouris et al., *Environ. Sci. Technol.*, 2011).

In neutron reflectometry (NR) experiments, theoretical calculations of the surface interaction potential between a particle and a flat silica surface using the DLVO theory were compared to the experimental data. The theory predicts that the potential energy is highly dependent on the ionic strength. In high ionic-strength solutions, NR reveals a high concentration of particles near the flat silica surface. Under the same conditions, theoretical calculations show an attractive force between a particle and a flat surface. For low ionic-strength solutions, the particle concentration near the surface obtained from NR is the same as the bulk concentration, while depletion of particles near the surface is expected because of the repulsion predicted by the DLVO theory. These results were presented at the 85th ACS Colloid and Surface Science Symposium held at McGill University in Montreal, Canada on June 19-22, 2011 and submitted for publication in a peer-reviewed journal.

In neutron imaging experiments, it was found that with no voltage applied, cations diffuse onto the outer zones of both electrodes. In another set of experiments, a DC voltage of 1.2 V was applied between the two electrodes. Under this potential, neutron-absorbing cations transported throughout the pores of the negatively charged electrode. From the comparison of the two time-series of images, we can infer that application of an electrical potential increases significantly the sorption capacity throughout the electrodes. The greater sorption capacity increases the driving force, so that transport through the electrodes is faster under an applied electrical potential. The concentration of neutron-absorbing ions adsorbed on the electrodes is directly proportional to the intensity of images according to the Beer-Lambert law. From the imaging data, the amount of neutron-absorbing ions adsorbed can be estimated as a function of time. The concentration profile of ions versus time can be used to estimate the diffusion coefficient of ions in the pores. Neutron imaging data can also be used to evaluate the predictive capabilities of transport models for ions in porous electrodes. Information about the diffusion coefficient can be utilized in devising material synthesis strategies for application in water desalination and energy storage. Furthermore, neutron imaging can be employed to study ion competition in counterbalancing the surface charge of the electrodes.

### **Training and Development:**

Graduate and undergraduate students, as well as postdoctoral fellows, worked on this project. Some of them collaborated with researchers in research laboratories (Oak Ridge National Laboratory). These interactions involved active participation and visits at the collaborator's site, often for extended periods of time.

Most of the students did both experimental and modeling work. Some had the opportunity to work more on experiments, others invested more in modeling, but they all supported their results with additional experimental and modeling work. Students had the opportunity to use modern experimental methods including Atomic Force Microscopy (AFM), cyclic voltammetry for electrical characterization of conductive surfaces, as well as neutron reflectometry and imaging.

A number of presentations related to the research of the project have been given at major conferences (Fifteenth Symposium on Separation Science and Technology for Energy Applications, Gatlinburg, TN, October 21-25, 2007; AIChE Annual Meeting, Salt Lake City, UT, November 4-9, 2007; 82nd ACS Colloid and Surface Science Symposium, North Carolina State University, Raleigh, NC, June 15-June 18, 2008; Chemical and Biological Defense Physical Science & Technology Conference, New Orleans, November 17-21, 2008; 13th International Conference and Surface and Colloid Science (ICSCS)/83rd ACS Colloid and Surface Science Symposium, Columbia University, New York City, NY, June 14-19, 2009; Sixteenth Symposium on Separation Science and Technology for Energy Applications, Gatlinburg, TN, October 18-22, 2009; Chemical and Biological Defense Physical Science & Technology Conference, Dallas, TX, November 16-20, 2009; 85th ACS Colloid and Surface Science Symposium, McGill University, Montreal, Quebec, Canada, June 19 ? 22, 2011; Seventeenth Symposium on

Separation Science and Technology for Energy Applications, Gatlinburg, TN, October 23-27, 2011; AIChE Annual Meeting, Minneapolis, MN, October 16-21, 2011) and several of them were delivered by students. The PI of the project was a member of the organizing committees for the Fifteenth, Sixteenth, and Seventeenth Symposia on Separation Science and Technology for Energy Applications and organized and chaired the sessions on 'Adsorption and Ion Exchange.' She also organized and chaired sessions in the AIChE Annual Meetings on 'Modeling of Interfacial Systems.'

The PI of the project co-authored the revision of Chapter 8 'Coagulation and Flocculation' of the 6th edition of Water Quality and Treatment, published by the American Water Works Association in 2010. The research of this project on understanding and quantifying interaction forces between colloidal particles and surfaces is very much related to the basic coagulation and flocculation processes employed in water treatment.

#### **Outreach Activities:**

Through this project, the PI had the opportunity to influence and recruit female students and researchers to pursue graduate studies and professional careers in environmental engineering. One example is Mary Lim, an excellent student in her undergraduate class, who was recruited by the PI to conduct undergraduate research through the project. The PI was also able to recruit three female graduate students (Eunhyea Chung, Ketki Sharma, and Hyojin Kewon) and a female postdoctoral fellow (Patricia Taboada-Serrano) in her research group.

#### **Journal Publications**

Hou, C. H., Taboada-Serrano, P., Yiacoumi, S., and Tsouris, C., "Monte Carlo Simulation of Electrical Double-Layer Formation from Mixtures of Electrolytes inside Nanopores", *Journal of Chemical Physics*, p. 044705, vol. 128, (2008). Published,

Hou, C. H., Wang, X. Q., Liang, C. D., Yiacoumi, S., Tsouris, C., and Dai, S., "Molecular-Sieving Capabilities of Nanoporous Carbon Materials", *Journal of Physical Chemistry B*, p. 8563, vol. 112, (2008). Published,

Taboada-Serrano, P., Vithayaveroj, V., Hou, C. H., Yiacoumi, S., and Tsouris, C., "Comparison between Effective Electrode/Electrolyte Interface Potential and Applied Potential for Gold Electrodes", *Industrial Engineering Chemistry Research*, p. 3525, vol. 47, (2008). Published,

Hou, C. H., Taboada-Serrano, P., Yiacoumi, S., and Tsouris, C., "Electrosorption Selectivity of Ions from Mixtures of Electrolytes inside Nanopores", *Journal of Chemical Physics*, p. 224703, vol. 129, (2008). Published,

Chung, E., Yiacoumi, S., Lee, I., and Tsouris, C., "The Role of the Electrostatic Force in Spore Adhesion", *Environmental Science & Technology*, p. 6209, vol. 44, (2010). Published,

Walker, M.E., McFarlane, J., Glasgow, D.C., Chung, E., Taboada-Serrano, P., Yiacoumi, S., and Tsouris, C., "Influence of Radioactivity on Surface Interaction Forces", *Journal of Colloid and Interface Science*, p. 595, vol. 350, (2010). Published,

Tsouris, C., Mayes, R. T., Kiggans, J., Sharma, K., Yiacoumi, S., DePaoli, D., and Dai, S., "Mesoporous Carbon for Capacitive Deionization of Saline Water", *Environmental Science & Technology*, p. , vol. , (2011). Published, 10.1021/es201551e

Chung, E., Yiacoumi, S., Halbert, C., Ankner, J., Wang, W., and Tsouris, C., "Interaction of Silica Nano-particles with a Flat Silica Surface Studied through Neutron Reflectometry", *Environmental Science & Technology*, p. , vol. , (2011). Submitted,

Chung, E., Yiacoumi, S., and Tsouris, C., "Interactions of Spores with Planar Surfaces in Aqueous Solutions", *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, p. , vol. , (2011). Submitted,

#### **Books or Other One-time Publications**

Letterman, R.D., and Yiacoumi, S., "Chapter 8, Coagulation and Flocculation", (2010). Book, Accepted

Editor(s): Edzwald, J. K.

Collection: Water Quality and Treatment, 6th edition

Bibliography: American Water Works Association, Denver, CO

Hou, C.-H., "Electrical Double Layer Formation in Nanoporous Carbon Materials", (2008). Thesis, Published Bibliography: Ph.D. Dissertation, Georgia Institute of Technology, Atlanta, GA

Chung, E., "Colloidal Particle-Surface Interactions in Atmospheric and Aquatic Systems", (2011). Thesis, Published Bibliography: Ph.D. Thesis, Georgia Institute of Technology, Atlanta, GA

### **Web/Internet Site**

### **Other Specific Products**

### **Contributions**

#### **Contributions within Discipline:**

The findings of this research provide a better understanding of various fundamental phenomena: (i) mechanisms of aggregation, breakup, and deposition of colloidal particles, nanoparticles, bacterial spores, and radioactive particles; (ii) influence of sorption of ionic pollutants on particle interactions; and (iii) interaction mechanisms of ionic species and porous nanostructured materials. These findings are significant in both engineered and natural environmental systems. They can be used in the design of processes for removing ionic and particulate pollutants from environmental systems and in quantifying transport and distribution of pollutants in natural environments.

#### **Contributions to Other Disciplines:**

The findings of this project are expected to contribute to a variety of separation and purification steps in the U.S. chemical industry, including separation and purification of nanomaterials, and lead to better ways to separate and purify precious metals, rare elements, and minerals, especially those that are lost in aqueous wastes of mining industries. Transport through porous materials and attachment to surfaces of inorganic, radioactive, and biological particles, including bacterial spores, viruses, and microorganisms, are basic functions that may be directly or indirectly linked to health and national security issues. The findings of this research will help provide solutions to such problems through isolation and inactivation of harmful inorganic, radioactive, and biological particles. The results of this study on the interaction of ionic species with nanostructured materials have important energy applications, such as energy storage in supercapacitors.

#### **Contributions to Human Resource Development:**

Courses were offered to students in Civil and Environmental Engineering at GIT. A unique feature of these courses is emphasis on mathematical modeling in environmental systems. Results from the research component of the project were incorporated into the lectures. Courses were offered through the Distance Learning Program of GIT and, therefore, reached industrial researchers and practitioners. In addition, research experience was provided to the students and postdoctoral fellows working on the project through visiting appointments at a National Laboratory. This project also gave the opportunity to the student and postdoc participants to pursue a future career in environmental engineering.

#### **Contributions to Resources for Research and Education:**

#### **Contributions Beyond Science and Engineering:**

### **Conference Proceedings**

#### **Categories for which nothing is reported:**

Any Web/Internet Site

Any Product

Contributions: To Any Resources for Research and Education

Contributions: To Any Beyond Science and Engineering

Any Conference